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Supplementary Information

The Reaction of Acetaldehyde, Glyoxal, and Ammonia to Yield 2-Methylimidazole: Thermodynamic and Kinetic Analyses of the Mechanism

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Schemes for the 2-methylimidazole formation Scheme A



















-NH3

CH₃

HO、

-H₂O

H₂N

-NH3 -CH₃ OH_PreIm -H₂O -CH₃















Scheme F



OH_noncyc_PreIm



OH_noncyc_PreIm









Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Х	-418.397340	-262548.31	-4.7
1.	-341.941343	-214571.44	5.7
2.	-418.394693	-262546.64	-3.1
OH_Pre_Im	-341.953040	-214578.78	-1.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S1. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme A).

Table S2. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme B).

proposed meenamon of 2 methymme	auzoie formation (b	eneme B).			
Structure	G, a.u.	G, kcal/mol	Gposition		
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0		
Water	-76.448667	-47972.26	0.0		
Ammonia	-56.563306	-35494.01	0.0		
Acetaldehyde	-153.850943	-96542.93	0.0		
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6		
1.1-ethanediol	-230.291459	-144510.08	-1.1		
1-aminoethanol	-210.403067	-132029.92	1.2		
ethanimine	-133.954955	-84058.01	6.7		
1.1-diaminoethane	-190.513636	-119549.12	3.8		
Bt_OHC-CHOHNH2	-284.442632	-178490.45	-5.7		
Bc_OHC-CHOHNH2	-284.440698	-178489.24	-4.5		
Y	-494.845299	-310520.13	-10.1		
X	-418.397340	-262548.31	-4.7		
Z	-474.956671	-298039.82	-8.0		
V	-398.507532	-250067.26	-1.9		
5	-418.393549	-262545.93	-2.3		
7	-418.386432	-262541.46	2.1		
2	-418.394693	-262546.64	-3.1		
OH_PreIm	-341.953040	-214578.78	-1.7		
OH_non_cyc_PreIm	-341.94197	-214571.83	5.3		
1	-341.941343	-214571.44	5.7		
6	-398.502137	-250063.88	1.5		
8	-398.497186	-250060.77	4.6		
3	-398.505197	-250065.80	-0.5		

NH2_PreIm	-322.067231	-202100.25	-1.4
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S3. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme C).

Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Cc_OHC-CHNH	-207.993268	-130517.75	0.5
Ct_OHC-CHNH	-207.991031	-130516.35	1.9
1	-341.941343	-214571.44	5.7
7	-418.386432	-262541.46	2.1
8	-398.497186	-250060.77	4.6
OH_Pre_Im	-341.953040	-214578.78	-1.7
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S4. The Gibbs free	e energies of the	structures in	solution	and the	PES	positions	of a	Ill structures	of	the
proposed mechanism of 2-	methylimidazole f	formation (Scl	neme D).							

	· · · · · · · · · · · · · · · · · · ·	,	
Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Dc_NH2HOHC-CHOHNH2	-341.006158	-213984.60	-11.7
Dt_NH2HOHC-CHOHNH3	-340.998213	-213979.62	-6.7
Y	-494.845299	-310520.13	-10.1
Z	-474.956671	-298039.82	-8.0
U	-474.958099	-298040.72	-8.9
W	-455.066935	-285558.82	-5.3
2.	-418.394693	-262546.64	-3.1

3.	-398.505197	-250065.80	-0.5
4.	-378.622770	-237589.39	-2.3
5.	-418.393549	-262545.93	-2.3
6.	-398.502137	-250063.88	1.5
7.	-418.386432	-262541.46	2.1
8.	-398.497186	-250060.77	4.6
9.	-378.613817	-237583.77	3.3
10.	-398.501704	-250063.61	1.7
OH_Pre_Im	-341.953040	-214578.78	-1.7
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_PreIm	-322.067231	-202100.25	-1.4
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S5. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme E).

Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Ec_NH2HOHC-CHNH	-264.549056	-166007.05	-0.6
Et_NH2HOHC-CHNH	-264.545815	-166005.01	1.4
5.	-418.393549	-262545.93	-2.3
6.	-398.502137	-250063.88	1.5
7.	-418.386432	-262541.46	2.1
8.	-398.497186	-250060.77	4.6
9.	-378.613817	-237583.77	3.3
OH_PreIm	-341.953040	-214578.78	-1.7
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_PreIm	-322.067231	-202100.25	-1.4
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S6. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme F).

Structure	G, a.u.	G, kcal/mol	Gposition		
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0		
Water	-76.448667	-47972.26	0.0		
Ammonia	-56.563306	-35494.01	0.0		

Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
Fc_HNHC-CHNH	-188.099923	-118034.49	5.5
Ft_HNHC-CHNH	-188.102608	-118036.17	3.8
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Reagents, TSs, products	TS	G, a.u	G, kcal/mol	$\Delta G^{\#}$, kcal/mol
cis-Glyoxal	~	-227.875282	-142993.9	
1.1-diaminoethane		-190.513636	-119549.1	
Water		-76.448667	-47972.3	
GO+NH2NH2CHCH3_X		-494.820826	-310504.8	3.0
Х	5	-418.39734	-262548.3	
Bc_OHC-CHOHNH2		-284.440698	-178489.2	
Water	ੱ پ	-76.448667	-47972.3	
1-aminoethanol		-210.403067	-132029.9	
Bc+OHNH2CHCH3_Y	.	-571.275241	-358480.6	3.3
Y	3 3 32	-494.845299	-310520.1	
Dc_NH2HOHC-CHOHNH2		-341.006158	-213984.6	
Acetaldehyde	- .	-153.850943	-96542.9	
Water		-76.448667	-47972.3	
Dc_Y	~~~	-571.272646	-358479.0	13.3
Y	J • •	-494.845299	-310520.1	
X		-418.39734	-262548.3	
Water		-76.448667	-47972.3	
X_2	<u>, 20</u>	-494.82611	-310508.1	5.0
2	3	-418.394693	-262546.6	
Y		-494.845299	-310520.1	
Water		-76.448667	-47972.3	
Y_2		-571.244764	-406413.6	23.4
2	- J	-418.394693	-262546.6	
2	<u></u>	-418.394693	-262546.6	
Water	ొలిం 🍦	-76.448667	-47972.3	
2_OH_PreIm	·•• • • •	-494.802258	-310493.1	18.3
OH_PreIm	1	-341.953040	-214578.8	
5	3.0 Q.3	-418.393549	-262545.9	
Water		-76.448667	-47972.3	
5_OH_PreIm		-571.228823	-358451.5	31.4
OH_PreIm	5	-341.953040	-214578.8	
OH_PreIm		-341.953040	-214578.8	
Water		-76.448667	-47972.3	
OH_PreIm_PreIm		-418.368062	-262529.9	13.6
PreIm		-265.518264	-166615.2	
PreIm		-265.518264	-166615.2	
Water		-76.448667	-47972.3	
PreIm_2MI		-341.921864	-214559.2	20.8
2MI	- 🍎 🖉	-265.552189	-166636.5	

Table S7. Transition states with the participation of one water molecule, and their Gibbs free energies and stage barriers for the mechanism of 2-methylimidazole formation



Identification of ¹H NMR signals in the spectra of reaction mixtures of 2MI formation with different orders of mixing of reagents

1 (blue) - Acetaldehyde \rightarrow Glyoxal \rightarrow Ammonia

2 (red) - Glyoxal \rightarrow Ammonia \rightarrow Acetaldehyde 3 (green) - Acetaldehyde \rightarrow Ammonia \rightarrow Glyoxal 4 (purple) - Water \rightarrow Glyoxal \rightarrow Ammonia 5 (yellow) - Water \rightarrow lack of THT \rightarrow Glyoxal 6 (orange) Water \rightarrow THT \rightarrow Ammonia \rightarrow Glyoxal 7 (light green) - Acetaldehyde \rightarrow lack of ammonia (3 h, 10 °C) \rightarrow Glyoxal 8 (black) - Acetaldehyde \rightarrow Ammonia (3 h, 10 °C) \rightarrow Glyoxal

Figure S1 shows the ¹H NMR spectra of the reaction mixtures of 2MI formation with different orders of mixing of the reagents at the end of the reaction. The chemical shift of the singlet signal of the protons of the internal standard (DMSO) is located in the region of 2.58 ppm. The protons of the methyl group of acetaldehyde feature a chemical shift of 1.22 ppm. The singlet of the protons of the methyl substituent in 2MI is detected at 2.21 ppm, and the signals of the methine protons of the imidazole ring of 2MI appear in a weak field (6.83 ppm). The spectral pattern of the reaction mixtures indicates the presence of additional signals in the regions of 3.53 ppm, 6.99 ppm, 7.63 ppm, 7.92 ppm, and 8.313 ppm, and these signals are related to the products of the competing reaction of glyoxal with ammonia. Singlet signal at 3.53 ppm is assigned to the protons of the CH_2 group of glycolic acid formed as a result of the Cannizzaro reaction, which was shown in our previous work³⁰. The signal at 6.99 ppm can be reliably assigned to the methine protons of the imidazole ring of hydrated imidazole-2-carbocaldehyde (HIC) since Ref.³² shows that similar protons of unhydrated imidazole-2-carbaldehyde (IC) appear in at 7.47 ppm. The 0.5 ppm shift is connected with the deactivation of the methine protons of the ring by the carbonyl group, which is characterized by a negative mesomeric effect that leads to a downfield shift of the signal, which is not observed in the case of the hydrated product. The remaining three signals in the weak field remain unidentified.



Fig. S2. Concentrations of the main products of the interaction of acetaldehyde, glyoxal, and ammonia in aqueous solution depending on the order of reagent mixing

Table S8. Concentrations of the main products, glyoxal conversion and selectivities towards the main products of the interaction of acetaldehyde, glyoxal, and ammonia in aqueous solution depending on the order of reagent mixing

N	Order of reagent mixing	C(HIC) C	C(GA),	C(2MI)	Total	Selectivity ² , %		, %	GO Goodala 3
0.	and their molar ratios	,М	M	, M	, M	HIC	GA	2MI	Conversion [*] , %
1	(Ac+GO)+2NH ₃	0.069	0.024	0.033	0.195	70.8	12.3	16.9	58.6
2	(GO+2NH ₃)+Ac	0.078	0.035	0.03	0.221	70.6	15.8	13.6	66.4
3	(Ac+2NH ₃)+GO	0.077	0.029	0.029	0.212	72.6	13.7	13.7	63.7
4	GO+2NH ₃	0.102	0.035		0.239	85.4	14.6	0.0	71.8
5	0.33THT+GO	0.007	0.015	0.062	0.091	15.4	16.5	68.1	27.3
6	0.33THT+NH ₃ +GO	0.031	0.012	0.092	0.166	37.3	7.2	55.4	49.8
7	(Ac+NH ₃)10 °C, 3h +GO	0.037	0.031	0.044	0.149	49.7	20.8	29.5	44.7
8	(Ac+2NH ₃)10 °C, 3h +GO	0.077	0.036	0.036	0.226	68.1	15.9	15.9	67.9

¹Total yield = $2 \cdot C(HIC) + C(GA) + C(2MI)$. 2 are because HIC formation requires 2 mol GO.

²Selectivity = $\frac{C_i}{Total \ yield} * 100.$ %. The concentration was multiplied by 2 in the case of HIC.

³ Conversion =
$$\frac{Total \ yield}{C(GO)_{initial}} * 100.\%$$

Structure	Atom	Х	Y	Z
	С	0.3291	0.6898	0.0000
	0	-0.3291	1.6986	-0.0001
	Н	1.4356	0.6728	0.0001
trans-Glyoxal (trans-GO)	С	-0.3291	-0.6898	0.0000
	0	0.3291	-1.6986	-0.0001
	H	-1.4356	-0.6728	0.0001
	0	0.0682	0.2921	-0.0000
Water	Н	0.8072	-0.2921	-0.0000
	Н	-0.8072	-0.0559	0,0000
	N	-0.0026	0.2314	-0.2007
	Н	-0.8094	0.7032	0.2006
Ammonia	Н	0.8094	0.6942	0.2006
	Н	-0.0078	-0.7032	0.2007
	C	0.4646	0.7632	-0.0006
	Н	0.5337	1 3728	-0.0001
	0	1 4692	-0.4100	-0.0008
Acetaldebyde	C	-0.9331	-0.2827	-0.0004
<i>rectandenyte</i>	Н	-1 4692	0.0926	-0 8784
	Н	-0.9225	-1 3728	-0.0009
	Н	-0.9225	0.0918	0.8784
		0.0000	0.7730	0.0704
	0	0.0000	-1.4018	-1.0120
	Ч	0.0000	1 2506	1.0120
cis-Glyoxal (cis-GO)		0.0000	0.7730	0.0136
	0	0.0000	1.4018	1.0120
	Ч	0.0000	1.4018	1.0120
		0.0000	0.4904	0.1442
	0	1 7/07	-0.4904	0.1442
	<u></u> Н	0.0531	1 5070	0.5773
	0	0.9331	1 3820	0.1804
	<u></u>	-0.0004	1.3820	-0.1804
B _c _OHC-CHOHNH ₂	N N	-1.5319	0.7741	-0.2300
		-1.5254	-0.7741	-0.4390
	П Ц	-1.1093	-1.0217	-1.3380
		-1.7497	-1.0270	0.0009
	Ц	-0.3749	0.0370	1 3586
		-0.8437	-0.0080	0.0000
	Ц	-0.2309	0.3880	0.0000
		-0.1424	0.2794	0.0000
C OHC CHNH	<u> </u>	2 1222	-0.3784	-0.0001
C _c Onc-Chivh	U U	0.0206	0.1373	0.0001
	п	1 2225	-1.4785	0.0001
		-1.3233	-0.2093	0.0000
		-2.1322	0.000	0.0001
		0.3103	-0.0310	1 4205
	П	0.4730	-0.0114	0.2457
		-0.0323	-0.0073	-0.3437
	п	-0.0782	-0.0019	-1.4293
	U U	-1.4420	1.2101	0.0090
		-2.2921	0.0702	-0.3390
		1.3921	-0.0723	-0.3388
		2.4023	-0.094/	0.2841
		-1.3001	-1.2033	0.0041
		-1.8413	-1.1/00	0.9803
	Н	-2.4023	-1.2964	-0.5552
		-0.2922	0.4439	0.0003
r _c _HNHU-UHNH	Н	-0.7098	1.4280	0.0000
		1.2077	0.4398	-0.0003

Table S9. Cartesian coordinates of the most stable states for all structures

	Н	1.6905	1.4189	-0.0002
	N	-0.9257	-0.6569	0.0000
	Н	-1 9345	-0 5022	-0.0002
	N	1.9345	-0.6026	-0.0003
	Н	1.3224	1.4286	0.0003
		0.6200	-1.4280	-0.0001
		-0.0299	-0.3027	-0.4334
	H	-0.7285	-1.0530	-1.2997
	<u> </u>	0.7616	0.2819	-0.51/4
	Н	0.8624	0.8347	-1.4568
	0	1.6663	-0.8420	-0.5066
	Н	2.5645	-0.5002	-0.4413
D NH.HOHC.CHOHNH.	0	-0.7423	-1.1070	0.7781
	Н	0.0216	-1.6993	0.8067
	Ν	-1.6500	0.6365	-0.5438
	Н	-2.5645	0.2108	-0.4339
	Н	-1.5206	1.3091	0.2072
	Ν	0.9321	1.2023	0.5761
	Н	0.8970	0.6985	1.4568
	Н	1 8136	1 6993	0 5179
	<u>г</u>	1 2090	-0.0026	-0.20/6
	н	1 7077	_0.8025	0.1814
		1.7077	-0.8925	0.1814
	П	1.7098	0.0003	1 2054
	H	1.2750	-0.0027	-1.2954
1.1-ethanediol HO(HO)CHCH ₃	<u> </u>	-0.2480	-0.0012	0.2015
	H	-0.3538	-0.0011	1.2954
	0	-0.8386	-1.1757	-0.3322
	Н	-1.7098	-1.2851	0.0646
	0	-0.8359	1.1742	-0.3321
	Н	-1.7072	1.2851	0.0641
	С	0.1492	0.3461	0.2296
	Н	0.1778	0.3934	1.3265
	0	0.6581	1.6146	-0.1785
	Н	0.7728	1.5579	-1.1363
	Ν	1.0052	-0.6958	-0.3269
1-aminoethanol HO(NH ₂)CHCH ₃	Н	1.9085	-0.6813	0.1376
_ (2) 5	Н	0.6033	-1.6146	-0.1669
	С	-1.2899	0.1432	-0.2335
	Н	-1 7069	-0.7869	0.1630
	Н	-1 9085	0.700	0.1071
	П	1 2227	0.1016	1 2265
	II N	-1.5257	0.1010	-1.5205
		-1.32/1	-0.3007	-0.0003
	П	-1.3822	-1.313/	-0.0007
		-0.4068	0.3003	-0.0003
Ethanimine NHCHCH ₃	H	-0.4346	1.3953	-0.0001
	С	0.9688	-0.3034	-0.0002
	Н	1.5271	0.0370	-0.8785
	Н	1.5267	0.0362	0.8785
	Н	0.9321	-1.3953	-0.0008
	C	0.2556	-0.0234	0.2282
	Н	0.2685	-0.0413	1.3297
	Ν	1.1016	-1.1415	-0.2054
	Н	0.7466	-2.0079	0.1902
	Н	1.0235	-1.2322	-1.2167
	N	0.8584	1.1959	-0.3221
1.1-diaminoethane_NH ₂ (NH ₂)CHCH ₃	H	0 3264	2,0079	-0.0224
	Н	1 7927	1 3015	0.0640
	 С	_1 2017	_0 11/12	_0.2360
	<u></u> и	-1.2017	1 0265	0.2300
	п u	-1.0003	-1.0303	0.1300
	Н	-1./92/	0.1297	0.1550
	Н	-1.2426	-0.1125	-1.3297

X C -2.3682 -9.6339 -0.0349 C -0.6040 -0.1981 0.0427 H -2.2094 -0.8555 1.0434 H -2.2094 -0.8555 1.0434 H -2.2094 -0.8555 1.0434 H -2.3756 0.7684 -1.3799 S -0.5528 -0.5710 -1.4526 H 2.0451 -1.179 -1.3526 H 1.9815 -1.179 -1.3526 H 0.6414 0.5710 -0.3528 O -1.7970 1.3462 0.5518 H 0.2017 1.4007 0.6823 O -2.7145 -1.7515 -0.7799 C -2.7255 0.6038 -1.4134 H -0.2145 -1.7515 -0.7799 C -2.7255 0.6038 -1.4134 H -2.7255 0.6038 -1.4134 H -2.7256 0.6038 -1.6134					
X C -1.6911 -0.4194 -0.330 C -0.6069 -0.1984 -1.3939 N -0.3520 0.1608 -1.0089 N -0.3520 0.01608 -1.0089 C 1.9989 -0.3528 0.5710 H -2.145 -0.6510 0.1986 H 1.2815 -1.1179 -1.3526 O -1.7970 1.3462 0.5518 H 0.6414 0.5710 0.8223 O -1.7970 1.3462 0.5518 H -0.015 0.99414 -1.5601 H -0.510 2.2098 0.0723 H 0.0218 -2.2098 0.0729 C -2.3550 -0.9245 -0.0208 C -1.7025 0.6683 -1.4134 N -0.3471 0.1673 -0.3244 C -0.0374 -0.0573 0.0198 H -2.2550 -0.6683 -1.4134		С	-2.3682	-0.8639	-0.0349
C 0.0609 -0.1981 0.0047 H -2.6794 -0.1885 1.0434 H -2.2736 0.7684 -1.3959 N -0.3520 0.1608 -1.0989 C 1.9589 -0.5288 -0.5710 H 2.27145 -0.6510 0.1986 H 2.3458 0.5808 +1.0122 H 0.2344 -0.5518 -0.5518 H 1.017970 1.3402 0.5518 H -0.0115 0.9414 -1.5601 O -1.7970 1.4007 0.6823 H 0.0271 -1.4007 0.6823 H 0.0514 -1.71515 -0.779 H 0.2345 -0.0245 0.0551 G -1.7023 0.3764 -0.5244 H -2.2550 0.0638 -1.4134 N 0.3071 0.1063 0.9572 H 2.0030 -1.1020 -1.36800 H		С	-1.6911	0.4194	-0.5350
X H -2.6094 -0.8885 1.0434 H -2.2736 0.7684 -1.3939 N -0.3520 0.10086 -1.0089 C 1.9989 -0.3528 0.5710 H 1.91815 -1.1179 -1.3526 H 1.9815 -1.0122 H 0.6414 0.5710 O -1.7770 1.3462 0.5518 H -0.611 0.9414 -1.5601 H -0.2028 -2.2098 0.0792 H 0.22145 -1.7155 4.02028 C -1.7203 0.3764 40.2344 H -2.2756 0.6638 -0.0511 H -2.2755 0.66723 0.1968 H -2.2755 0.66723 0.1968 H 2.2089 0.0271 -1.408 K H 2.2081 0.2029 H 2.0375 0.6632 -0.9752 C 0.0312 0.5629		С	0.6069	-0.1981	0.0427
X H -2.2736 0.7684 -1.9399 N -0.3528 -0.5710 -1.0689 -0.3528 -0.5710 H 2.7145 -0.6510 0.1986 -0.1986 H 2.3458 0.5508 -1.0179 -1.3525 O -1.7970 1.3462 0.5518 H 0.0208 -2.2098 0.2354 H 0.0217 -1.0077 -6.0077 H 0.0218 -0.2098 0.2354 H 0.0208 -2.2098 0.0792 H 0.0514 -1.7515 -0.7799 C -2.3550 -0.9245 -0.0208 C -0.17023 0.3764 -0.3204 C 0.0138 -0.0458 -0.0511 H -2.2795 -0.6723 0.0792 H -2.3500 -0.9459 1.0073 H 2.0030 -1.1020 -1.3680 H 2.0300 -1.020 -1.3680 H <th></th> <th>Н</th> <th>-2.6094</th> <th>-0.8585</th> <th>1.0434</th>		Н	-2.6094	-0.8585	1.0434
X 0.3320 0.1668 -1.0099 C 1.9989 -0.3528 0.05710 H 2.145 -0.6610 0.1986 H 1.9815 -1.1179 -1.3526 H 2.3458 0.5868 -1.0122 H 0.6414 0.5710 0.8233 O -1.7970 1.3462 0.5518 H -0.0115 0.9414 -1.5601 H -0.5514 -1.5610 0.2384 N 0.0777 -1.4007 0.6823 H 0.2028 -2.2098 0.0234 O -2.2145 1.0209 -0.3248 C -1.7023 0.3764 -0.524 H 2.2550 -0.9245 -0.0208 C -1.0123 0.0563 -0.4733 H 2.2550 -0.6723 0.1968 H 2.2051 0.6638 -0.2028 C 2.0639 -0.4163 -0.5239 H		Н	-2.2736	0.7684	-1.3959
X X X X X X X X X X		N	-0.3520	0 1608	-1.0089
X H L 27145 -0.6510 -0.1986 -0.1179 -1.3326 H L 27145 -0.6510 -0.1986 -1.1179 -1.3326 -1.342 -0.5118 H -0.414 -0.5710 -0.8253 -0 -1.777 -1.4007 -0.6823 H -0.0115 -0.9414 -1.501 -1.2098 -0.2354 N -0.0277 -1.4007 -0.6823 H -0.2355 -0.028 -2.208 0.0792 H -0.2355 -0.0245 -0.0294 -0.0218 -0.2354 -0.0294 -0.0218 -0.2354 -0.0294 -0.0218 -0.235 -0.024 -0.0218 -0.235 -0.024 -0.0218 -0.235 -0.024 -0.0218 -0.024 -0.0218 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.024 -0.021 -0.021 -0.022 -0.025		C	1 9989	-0.3528	-0.5710
X H L L L H L L L L H L L L H L L L L L H L L L L L L H L		<u>с</u> ц	2 7145	-0.5520	0.1086
X H H H H H H H H H H H H H H H H H H H			2.7145	-0.0310	1.2526
Y H 0.414 0.5710 0.8253 0 -1.7970 1.3462 0.5518 H -0.0115 0.9414 -1.5601 H -0.0177 -1.4007 0.6823 N 0.0777 -1.4007 0.6823 H 0.2028 -2.2098 0.0792 H 0.0514 -1.5840 1.5601 O -2.7145 -1.7315 -0.7799 C -2.3550 -0.9245 -0.0208 C -0.6138 -0.2458 0.0551 H -2.2755 0.66638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0639 -0.6123 0.06621 H 2.0205 -0.6723 0.1066 C 2.0305 -1.7023 0.3764 H 2.0305 -1.723 0.5729 H 2.0430 -1.1020 -1.3780 N 0.1093 -1.4768 0.6621 <	Х	П	1.9013	-1.11/9	-1.5520
H 0.0414 0.5710 0.8253 O -1.7970 1.3462 0.5518 H -0.0115 0.9414 -1.5601 H -0.0128 -2.2098 0.0792 H 0.0514 -1.5840 1.5601 O -2.7145 -1.7515 -0.7799 C -2.3550 -0.9245 -0.0208 C -1.7023 0.3764 -0.5204 C 0.6138 -0.2458 0.05511 H -2.2550 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0389 -0.3612 -0.5629 H -2.2725 -0.6673 0.19752 H 0.6370 0.4999 0.8399 H -0.6101 0.9106 -1.5256 O -2.7243 -1.8018 -0.7680 N 0.1093 -1.4768 0.6621 H 0.2377 -2.021 0.0291 H		Н	2.3458	0.5868	-1.0122
V -1.797.0 1.3462 0.5518 H -0.0115 0.9414 -1.5601 H -0.0115 0.2098 0.2354 N 0.0777 1.4007 0.6823 H 0.2028 -2.2098 0.0792 H 0.5514 -1.5810 1.5715 H 0.27145 -1.7515 -0.7799 C -2.3550 0.9245 -0.0208 C 0.6138 -0.2458 0.0351 H -2.2755 0.6638 -1.4134 N 0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.7295 -0.66723 0.1968 C 2.0089 -0.3612 -0.5629 H 2.0030 -1.1020 -1.3680 H 0.2037 -2.2621 0.0291 H 0.6302 1.5256 0 O -2.7243 -1.8018 -0.7680 H -		H	0.6414	0.5/10	0.8253
H -0.0115 0.9414 -1.5601 H -0.15101 2.2098 0.0792 H 0.0514 -1.5840 1.5601 O -2.7145 -1.7515 -0.7799 C -2.3550 -0.9245 -0.0208 C -1.7023 0.3764 -0.5204 C -0.138 -0.2458 0.0551 H -2.5540 -0.9549 1.0673 H -2.033 0.3612 -0.5629 H -0.3721 0.1663 -0.9916 C 2.0030 -1.1020 -1.3680 H -0.0337 -1.3640 0.621 H 0.6370 0.9999 0.8599 H -0.0101 0.9106 -1.5256 N		0	-1.7970	1.3462	0.5518
H -1.5101 2.2098 0.2354 H 0.2028 -2.2098 0.0792 H 0.2028 -2.2098 0.0792 H 0.5514 -1.5840 1.5601 O -2.7145 -1.7515 -0.7799 C -2.3550 -0.9245 -0.0208 C 0.6138 -0.2458 0.0551 H -2.2540 -0.549 1.0673 H -2.2575 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0609 -0.3612 -0.5629 H 2.7295 0.6638 -1.4134 N -0.3912 -0.6621 0.0565 C 2.0030 -1.1020 -1.3680 H 2.0320 0.5965 -0.9752 H 0.6370 0.4999 0.8599 H -0.21743 -1.8018 -0.7680 N 0.1093 -1.4768 0.6621 H		H	-0.0115	0.9414	-1.5601
N 0.0777 -1.4007 0.6823 H 0.2028 -22098 0.0792 H 0.5514 -1.5840 1.5601 O -2.7145 -1.7515 -0.7799 C -2.3550 -0.9245 -0.0208 C -1.7023 0.3764 -0.5204 C 0.6138 -0.2458 0.0051 H -2.2550 -0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.2795 -0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.0030 -1.1020 -1.3680 N 0.1093 -1.4768 0.6621 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.2091 1.5439 0.8234 C		Н	-1.5101	2.2098	0.2354
H 0.2028 -2.2098 0.0792 H 0.5514 -1.5840 1.5601 O -2.7145 -1.7515 -0.7799 C -2.3550 -0.9245 -0.0208 C -1.7023 0.3764 -0.5204 C 0.6138 -0.2458 0.0551 H -2.2755 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0375 -0.6723 0.1968 H 2.0300 -1.1020 -1.3680 H 2.0300 -1.1020 -1.5256 O -2.7243 -0.6723 0.01968 H -0.0101 0.9106 -1.5256 O -2.7243 -1.8018 -0.6621 H 0.6300 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.1402 1.3752 0.5570 H -1.4095 2.2621 0.0397 C		N	0.0777	-1.4007	0.6823
H 0.5514 -1.5840 1.5501 O -2.7145 -1.7515 -0.7799 C -2.3550 -0.9245 -0.0208 C -1.7023 0.3764 -0.5204 C 0.6138 -0.2458 0.0551 H -2.2550 -0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.7295 -0.6723 0.1968 H 2.0030 -1.1020 -1.3680 N 0.1570 0.4999 0.8599 H -0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.6300 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.5439 0.8234 C 0.5955 2.0577 -0.0597 H -1.4095 2.2621 0.2078 H		Н	0.2028	-2.2098	0.0792
O -2.7145 -1.7151 -0.7799 C -2.3550 -0.9245 -0.0208 C -1.7023 0.3764 -0.5204 C 0.6138 -0.2458 0.0551 H -2.5540 -0.9549 1.0673 H -2.2755 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.0030 -1.1200 -1.3680 H 2.0300 -1.1200 -1.3680 H 0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.0600 -1.5252 0.5700 H 0.0600 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.622 1.3752 0.5700 H -1.4095 2.2621 0.2078 C 0.3379 1.3041 0.9241 C		Н	0.5514	-1.5840	1.5601
C -2.3550 -0.9245 -0.0008 C -1.7023 0.3764 -0.5204 C 0.6138 -0.2458 0.0551 H -2.2550 0.6038 -1.4134 N -0.3471 0.1163 -0.9916 C 2.00089 -0.3612 -0.5629 H 2.7275 -0.6733 0.1968 H 2.0300 -1.1020 -1.3680 H 2.0370 0.4999 0.8599 H 2.0370 0.4999 0.8599 H -0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7213 -1.4768 0.6621 H -2.4221 0.0597 0.570 H -2.7233 -1.6332 1.5256 O -2.7243 -1.6133 0.8234 C <		0	-2.7145	-1.7515	-0.7799
C -1.7023 0.3764 -0.5204 C 0.6138 -0.2488 0.0551 H -2.5540 -0.9549 1.0673 H -2.2755 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.2023 -0.1023 0.1968 H 2.0030 -1.1020 -1.3680 H 2.0030 -0.1023 0.1968 H 2.0030 -1.1020 -1.3680 H 2.0030 -1.4768 0.6621 H 0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.6000 1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -2.7295 1.5439 0.8234 C 0.35955 2.0577 -0.0597 C <		С	-2.3550	-0.9245	-0.0208
C 0.6133 -0.2458 0.0551 H -2.5540 -0.9549 1.0673 H -2.2755 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.725 -0.6723 0.1968 H 2.0030 -1.1020 -1.3680 H 2.0303 -0.1010 0.9106 -1.5256 H 0.6370 0.4999 0.8399 H 0.0103 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -2.7233 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 C 0.5955 2.0577 -0.0597 C -0.3379 1.3041 0.9241		С	-1.7023	0.3764	-0.5204
H -2.5540 -0.9549 1.0673 H -2.2755 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.7295 -0.6723 0.1968 H 2.0300 -1.1020 -1.3680 H 2.0370 0.4999 0.8399 H 0.6370 0.4999 0.8399 H 0.6070 0.4999 0.8399 H 0.20387 -2.2621 0.0291 H 0.20387 -2.2621 0.0297 H -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.3595 2.0577 -0.0597 C 0.3359 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4		С	0.6138	-0.2458	0.0551
H -2.2755 0.6638 -1.4134 N -0.3471 0.1163 -0.9916 C 2.0089 -0.3612 -0.5629 H 2.7295 -0.6723 0.1968 H 2.0300 -1.1020 -1.3680 H 2.3420 0.5965 -0.9752 H 0.6370 0.4999 0.8599 H -0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.68970 N		Н	-2.5540	-0.9549	1.0673
N -0.3471 0.1163 -0.0916 C 2.0089 -0.3612 -0.5629 H 2.7295 -0.6723 0.1968 H 2.0300 -1.1020 -1.3680 H 2.0303 -1.1020 -1.3680 H 0.6370 0.4999 0.8599 H 0.6370 0.4999 0.8599 H 0.0310 0.1000 -1.5256 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -1.4095 2.2621 0.2078 H -1.4037 1.3041 0.9241 C 0.3595 2.0577 -0.0597 C -0.3379 1.3041 0.9241 C 0.		Н	-2.2755	0.6638	-1.4134
V C 2.0089 -0.3612 -0.5629 H 2.7295 -0.6723 0.1968 H 2.0300 -1.1020 -1.3680 H 2.0420 0.5965 -0.0752 H 0.6370 0.4999 0.8599 H -0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 N 0.3166 1.6662 -1.4376 H 0.2224 1.7957 1.8970 N 0.0202 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H<		N	-0.3471	0.1163	-0.9916
V H 2.7295 -0.6723 0.1968 H 2.0300 -1.1020 -1.3580 H 2.3420 0.5965 -0.9752 H 2.3420 0.5965 -0.9752 H 0.6370 0.4999 0.8599 H 0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.16022 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.3379 1.3041 0.9241 C 0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.2685 H		С	2.0089	-0.3612	-0.5629
V H 2.0030 -1.1020 -1.3680 H 2.3420 0.5965 -0.9752 H 0.6370 0.4999 0.8599 H 0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H 0.2224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H 0.4142 -2.7314 1.4590 H <th></th> <th>H</th> <th>2.7295</th> <th>-0.6723</th> <th>0.1968</th>		H	2.7295	-0.6723	0.1968
V H 2.3320 0.5965 -0.9752 H 0.6370 0.4999 0.8599 H -0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.5955 2.0577 -0.0597 C 0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H <th></th> <th>Н</th> <th>2.0030</th> <th>-1 1020</th> <th>-1 3680</th>		Н	2.0030	-1 1020	-1 3680
H D.101 0.4999 0.8399 H 0.6370 0.4999 0.8399 H 0.0101 0.9106 -1.5256 N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -2.7295 1.5439 0.8234 C 0.5955 2.0577 -0.0597 C -0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H 0.43450 -3.1299 -0.2685 H 0.107	V	Н	2.3420	0 5965	-0.9752
H 0.0101 0.0103 0.14768 0.6621 N 0.1093 -1.4768 0.6621 0.0291 H 0.0600 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8344 C 0.5955 2.0577 -0.0597 C 0.3379 1.3041 0.9241 C 0.3343 -1.1011 0.1458 N 0.3166 1.6662 -1.4376 H -0.224 1.7957 1.8970 N -0.0254 -2.4458 0.4969 H 0.4348 3.1299 -0.2685 H 0.4142 -2.7314 1.4590 C -0.0254 -2.4458 0.4969 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 <	·	Н	0.6370	0.4999	0.8599
N 0.1093 -1.4768 0.6621 H 0.2387 -2.2621 0.0291 H 0.6000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.3379 1.3041 0.9241 C 0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.8970 N -0.0254 -2.4458 0.4969 H 0.4142 -3.1299 -0.2685 H 0.4142 -2.7314 1.4590 O 1.9516 1.8281 0.2599 O 1.9516 1.8281 0.2599 H -0.6811		Н	-0.0101	0.9106	-1 5256
Y Image: height of the system I		N	0.1093	-1 4768	0.6621
Y H 0.0000 -1.6832 1.5256 O -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.5955 2.0577 -0.0597 C -0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H -0.2224 1.7957 1.8970 H -0.2224 1.7957 1.8970 N -0.0254 -2.4458 0.4969 H 0.4348 3.1299 -0.2685 H 0.4142 -2.7314 1.4590 C -0.0254 -2.4458 0.4969 H -0.1077 -0.7025 -0.7229 O 1.9516 1.8281 0.2509 H -0.1077 -0.7025 -0.7292 <td< th=""><th></th><th>Н</th><th>0.2387</th><th>2 2621</th><th>0.021</th></td<>		Н	0.2387	2 2621	0.021
Y In 0.0000 -1.03.2 1.2.33 0 -2.7243 -1.8018 -0.7680 N -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.3955 2.0577 -0.0597 C 0.3343 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.8970 N -0.0254 -2.4458 0.4969 H 0.43450 -3.1299 -0.2685 H 0.4142 -2.7314 1.4590 O 1.9516 1.8281 0.2509 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H -0.66811 1.7458 -1.6093 O 1.9516 1.8281 0.2509		 Ц	0.2387	-2.2021	1.5256
Y O -1.7622 1.3752 0.5570 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.5955 2.0577 -0.0597 C -0.3379 1.3041 0.9241 C 0.3166 1.6662 -1.4376 H -0.2224 1.7957 1.8970 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H 0.4142 -2.7314 1.4590 H 0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H 2.1028 0.8801 0.0697 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H <th></th> <th>0</th> <th>0.0000</th> <th>-1.0052</th> <th>0.7690</th>		0	0.0000	-1.0052	0.7690
Y -1.1022 1.372 0.3370 H -1.4095 2.2621 0.2078 H -2.7295 1.5439 0.8234 C 0.5955 2.0577 -0.0597 C -0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H 0.3450 -3.1299 -0.2685 H 0.4142 -2.7314 1.4590 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H 2.1028 0.8801 0.0697 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H 2.02		U N	-2.7243	-1.0010	-0.7080
H -1.4093 2.261 0.2078 H -2.7295 1.5439 0.8234 C 0.5955 2.0577 -0.0597 C -0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H 0.3450 -3.1299 -0.2685 H 0.4142 -2.7314 1.4590 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H 2.1028 0.8801 0.0697 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H 2.1028 0.8801 0.0697 H -0.23			-1.7022	2.2621	0.3370
H -2./293 1.3439 0.8234 C 0.5955 2.0577 -0.0597 C -0.3379 1.3041 0.9241 C 0.3453 -1.0111 0.1458 N 0.3166 1.6662 -1.4376 H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H 0.3450 -3.1299 -0.2685 H 0.4142 -2.7314 1.4590 H 0.4142 -2.7314 1.4590 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H 2.1028 0.8801 0.0697 H -0.6811 1.7458 -1.6093 O -1.6629 1.5060 0.4216 H 0.3376 -0.2770 2.0675 H 2.2		П	-1.4093	2.2021	0.2078
$\begin{array}{c cccc} C & 0.3953 & 2.0577 & -0.0397 \\ \hline C & -0.3379 & 1.3041 & 0.9241 \\ \hline C & 0.3453 & -1.0111 & 0.1458 \\ \hline N & 0.3166 & 1.6662 & -1.4376 \\ \hline H & 0.4348 & 3.1299 & 0.1199 \\ \hline H & -0.2224 & 1.7957 & 1.8970 \\ \hline N & -0.0920 & -0.1011 & 1.1692 \\ \hline C & -0.0254 & -2.4458 & 0.4969 \\ \hline H & 0.3450 & -3.1299 & -0.2685 \\ \hline H & 0.4142 & -2.7314 & 1.4590 \\ \hline H & -1.1090 & -2.5473 & 0.5750 \\ \hline H & -0.1077 & -0.7025 & -0.7929 \\ \hline O & 1.9516 & 1.8281 & 0.2509 \\ \hline H & 2.1028 & 0.8801 & 0.0697 \\ \hline H & -0.6811 & 1.7458 & -1.6093 \\ \hline O & -1.6629 & 1.5060 & 0.4216 \\ \hline H & 0.3376 & -0.2770 & 2.0675 \\ \hline H & -2.2358 & 0.9212 & 0.9310 \\ \hline O & 1.7784 & -0.9316 & -0.1230 \\ \hline H & 0.7911 & 2.3055 & -2.0675 \\ \hline H & 2.2358 & -1.3771 & 0.6016 \\ \hline C & 0.9933 & 0.6944 & 1.0664 \\ \hline \end{array}$		Н	-2.7295	1.5439	0.8234
$Y \qquad \qquad$		C C	0.5955	2.0577	-0.0597
$Y \qquad \qquad$		<u> </u>	-0.3379	1.3041	0.9241
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		<u> </u>	0.3453	-1.0111	0.1458
H 0.4348 3.1299 0.1199 H -0.2224 1.7957 1.8970 N -0.0920 -0.1011 1.1692 C -0.0254 -2.4458 0.4969 H 0.3450 -3.1299 -0.2685 H 0.4142 -2.7314 1.4590 H -1.1090 -2.5473 0.5750 H -0.1077 -0.7025 -0.7929 O 1.9516 1.8281 0.2509 H 2.1028 0.8801 0.0697 H -0.6811 1.7458 -1.6093 O -1.6629 1.5060 0.4216 H 0.3376 -0.2770 2.0675 H 2.2358 0.9212 0.9310 O 1.7784 -0.9316 -0.1230 H 0.7911 2.3055 -2.0675 H 2.2358 -1.3771 0.6016 C 0.9933 0.6944 1.0664 C 1.4		N	0.3166	1.6662	-1.4376
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$		H	0.4348	3.1299	0.1199
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		H	-0.2224	1.7957	1.8970
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		N ~	-0.0920	-0.1011	1.1692
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		<u>C</u>	-0.0254	-2.4458	0.4969
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		Н	0.3450	-3.1299	-0.2685
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		Н	0.4142	-2.7314	1.4590
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Y	Н	-1.1090	-2.5473	0.5750
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		Н	-0.1077	-0.7025	-0.7929
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		0	1.9516	1.8281	0.2509
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		Н	2.1028	0.8801	0.0697
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		Н	-0.6811	1.7458	-1.6093
H 0.3376 -0.2770 2.0675 H -2.2358 0.9212 0.9310 O 1.7784 -0.9316 -0.1230 H 0.7911 2.3055 -2.0675 H 2.2358 -1.3771 0.6016 C 0.9933 0.6944 1.0664 C 1.4689 -0.7958 1.0602		0	-1.6629	1.5060	0.4216
H -2.2358 0.9212 0.9310 O 1.7784 -0.9316 -0.1230 H 0.7911 2.3055 -2.0675 H 2.2358 -1.3771 0.6016 C 0.9933 0.6944 1.0664 C 1.4689 -0.7958 1.0602		Н	0.3376	-0.2770	2.0675
O 1.7784 -0.9316 -0.1230 H 0.7911 2.3055 -2.0675 H 2.2358 -1.3771 0.6016 C 0.9933 0.6944 1.0664 C 1.4689 -0.7958 1.0602		Н	-2.2358	0.9212	0.9310
H 0.7911 2.3055 -2.0675 H 2.2358 -1.3771 0.6016 C 0.9933 0.6944 1.0664 C 1.4689 -0.7958 1.0602		0	1.7784	-0.9316	-0.1230
H2.2358-1.37710.6016C0.99330.69441.0664C1.4689-0.79581.0602		Н	0.7911	2.3055	-2.0675
Z C 0.9933 0.6944 1.0664 C 1.4689 -0.7958 1.0602		Н	2.2358	-1.3771	0.6016
L C 1.4689 -0.7958 1.0602	7	С	0.9933	0.6944	1.0664
	L	С	1.4689	-0.7958	1.0602

	С	-0.9240	0 7488	-0 5321
	N	0.7243	1 1842	0.1746
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	H	2.4205	-0.8372	1.6011
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	Н	-2.4205	1.2703	-2.0150
	Н	-1 5688	1.0081	0.3181
	<u> </u>	2 1401	1.0001	1 2620
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	H	1.9046	2.3855	1.1849
	H	1.0662	0.9631	-0.9337
	H	-1.8050	-0.9395	-1.3522
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		0.9000	-1.241/	0.7271
		-0.0029	0.0001	0.3313
		-1./685	-0.4/31	0.9466
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	Н	2.3220	0.5501	0.8048
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XX /	П	2.3182	-0.4077	-2.3193
W	H	0.1907	0.2844	-1.8/2/
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č	н	-0.4051	3 6188	0.1554
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	N	1.1760	-1.6615	-1.1238
	Н	0.7482	-1.7706	-2.0409
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	C	-1 9906	0 1615	0 2426
	C	-1.0965	-1.0256	-0.0170
	C	1.0705	-0.0718	-0.4076
	U N	0.6799	1 2001	-0.4070
		1.6746	1.2901	-0.0990
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	N C	0.1401	-1.1323	-0.2871
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	H	2.1095	-0.5391	1.4697
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		1.0413	0.0789	0.3008
	C	1.0027	-0.0888	-0.5289
		-1.1028	-0.1343	0.4083
		-0.3040	1.1118	0.3048
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	N	-0.2534	-1.2801	0.1524
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	Н	-0.5283	1.5325	-0.5483
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	N	2.1314	-1.0423	-0.7988
	Н	2.8406	0.3171	0.6968
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	н	-2.8880	-1 5792	0.3390
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	Н	2.9468	-1.6374	-0.6783
	Н	2.3053	-0.4468	-1.6044
	0	-0.3646	-1.8304	-0.1426
	H	0.4632	-1 7818	-0 6794
	C II	0.8282	-1.0773	_0 2899
	C C	1 2045	0.0221	0.2077
	<u> </u>	1.0745	-0.0221	-0.0012
		-1.2373	0.1628	-0.4145
	N	-0.4374	-1.0490	-0.1795
	Н	1.2936	-2.0492	-0.0874
	Н	2.5312	-0.4486	-1.3841
	Ν	-0.7825	1.2582	0.4730
	C	-2.7098	-0.1980	-0.2244
	Н	-2.9970	-0.9955	-0.9142
6	Н	-2.8796	-0.5491	0.7976
	Н	-3.3484	0.6696	-0.4105
	Н	-1.0767	0.5084	-1 //13
	и П	1.0707	2 0402	0.2083
		-1.41//	0 1757	0.3703
	IN IN	2.1001	0.1/5/	0.3792
	H	2.1813	0.2825	1.4131
	H	3.3484	-0.6340	0.7317
	0	1.4093	1.1983	-1.0921
	Н	0.7289	1.4970	-0.4415
	Н	-0.8191	0.9464	1.4413
	С	1.3080	-0.2011	-0.3876
	C	1.5867	1.0654	0.4224
	C	-1 2375	-0 3977	-0.1476
7		0.0152	0.3777	0.1470
		-0.0133	-0.4720	-0.070/
	H	1.9433	-0.1144	-1.2821
	H	2.5931	1.0603	0.8544

	N	0.8520	2 0803	0 5082
	N G	0.6520	2.0605	0.3982
	C	-1.1078	-0.8644	1.2974
	Н	-0.7307	-1.8864	1.3387
	Н	-0.4295	-0.2195	1.8560
	Ч	2 0807	0.8315	1 7752
		-2.0697	-0.0313	0.6602
	H	-1.9642	-1.0312	-0.6693
	0	1.7873	-1.2661	0.4378
	Н	1.6316	-2.0803	-0.0551
	Н	-0.1366	-0 1811	-1 8560
	0	1 7444	0.0650	0.2084
	<u> </u>	-1.7444	0.9039	-0.2004
	Н	-2.5931	0.9987	0.2501
	Н	-0.0680	1.9388	0.1648
	С	1.3309	-0.1936	-0.4142
	С	1.6023	1.0881	0.3761
	С	-1 2252	-0.4510	-0 1335
	N	0.0132	0.5216	0.8083
		1.0510	-0.3210	-0.8983
	H	1.9510	-0.1045	-1.3199
	H	2.6430	1.1319	0.7190
	N	0.8333	2.0599	0.6298
	С	-1.0555	-0.9134	1.3113
	Н	-0.6209	-1.9120	1.3423
Q	и П	_0 4052	_0.2365	1 8666
0	11	-0.4032	-0.2303	1.8000
	H	-2.0305	-0.9378	1.8039
	H	-1.9088	-1.1491	-0.6348
	0	1.8588	-1.2348	0.4202
	Н	1.6796	-2.0599	-0.0461
	Н	-0 1153	-0 2647	-1 8666
	Ч	0.1204	1 8685	0 2705
	11 N	1 7097	0.0197	0.2795
	N	-1./98/	0.9187	-0.1470
	H	-2.0874	1.1535	-1.0935
	Н	-2.6430	0.9462	0.4204
	С	-1.3941	-0.6154	0.3102
	С	-2.0462	0.7623	0.4104
	C	1 0272	-0.0016	0.2543
		0.1276	-0.0010	0.4142
	IN IN	-0.1270	-0.0073	-0.4145
	H	-1.2/88	-0.98/3	1.3441
	Н	-3.0264	0.7192	0.9029
	Ν	-1.6332	1.8812	-0.0182
	С	2.2121	-0.9730	0.2522
	Н	1.9775	-1.8812	0.8152
	Н	2 /629	-1.2545	-0.7761
9	II	2.4027	0.5061	0.7/01
		0.7720	-0.3001	1.2056
	H	0.7728	0.2368	1.2956
	Н	0.0672	-1.5692	-0.6645
	N	-2.2748	-1.5676	-0.3784
	Н	-3.0917	-1.7681	0.1898
	Н	-2.6085	-1.1555	-1.2464
	N	1 3237	1 2879	-0 3992
	Ц	2.0752	1.2075	0.0021
	П	2.0732	1.7040	0.0931
	H	1.6558	1.10/8	-1.3441
	Н	-0.6875	1.7880	-0.4180
	С	-1.3996	-0.5742	0.2572
	С	-2.0259	0.8161	0.3346
	С	1.0214	-0.0149	0.2116
	N	_0 1205	-0 5715	-0.4586
10	TT	1 2029	-0.3713	1 2009
10	н	-1.2928	-0.9434	1.2908
	H	-2.9586	0.8346	0.9100
	<u>N</u>	-1.6308	1.8877	-0.2164
	С	2.2161	-0.9604	0.1598
	Н	2.0008	-1.8877	0.6972
				· · · · · -

	Н	2.4494	-1.1955	-0.8824
	Н	3.0939	-0.4940	0.6117
	Н	0.7717	0.2129	1.2578
	Н	0.0419	-1 5081	-0.8007
	N	_2 2884	-1 51/3	-0.4347
	н	3 0030	1.5145	0.1/32
	<u>п</u>	2 6380	1.0012	1 2008
	П	-2.0380	-1.0912	-1.2908
	П	-0.7598	1.7190	-0.0972
	0	1.3405	1.2270	-0.4544
	H	1.9545	1./1/3	0.1122
	C	-1.4013	-0.2091	0.4526
	C	-0.8269	1.0804	-0.0983
	C	0.9504	-0.0934	0.5211
	N	-0.2346	-0.7320	1.1309
	Н	-2.2423	-0.0686	1.1387
	Н	-1.4488	1.8568	-0.5346
	N	0.4419	1.1363	-0.1025
OH_PreIm	C	1.6768	-0.9513	-0.5184
	Н	2.0697	-1.8568	-0.0488
	Н	0.9792	-1.2379	-1.3085
	Н	2.5113	-0.3999	-0.9576
	Н	1.6536	0.1982	1.3085
	0	-1.8503	-0.9681	-0.6861
	Н	-2.5113	-1.5984	-0.3805
	Н	-0.2030	-1.7445	1.1257
	С	-1.2148	-0.2231	0.5195
	С	-0.6348	1.0552	-0.0608
	C	1.1697	-0.1102	0.5091
	N	0.0072	-0.8954	0.9817
	Н	-1.8985	-0.0095	1.3496
	Н	-1 2667	1 8450	-0.4620
	N	0.6326	1 1115	-0.1151
	C	2 0752	-0.8667	-0.4604
NH2_PreIm	Н	2.0732	-1 7696	0.0148
	Н	1 51/8	-1 1560	-1 3539
	Ц	2 0188	0.2418	0.7616
	<u>п</u>	1.7675	-0.2410	1 3687
		0.0204	1.8450	0.6279
	П	1.0626	-1.0430	0.0278
	IN II	-1.9030	-1.0550	-0.4407
	П	-2.9188	-0.0994	-0.3317
	H	-1.558/	-0.9737	-1.308/
		-0.9684	0.8884	-0.3641
	Н	-1.3842	1.8330	-0.9245
		-2.0156	-0.0//1	-0.1145
	H	-2.9622	0.3914	0.1730
	N	-1.8412	-1.3385	-0.0985
	H	-2.6705	-1.8330	0.2303
	N ~	0.2999	0.7876	-0.5534
OH_noncycPreIm	C	0.9625	-0.4389	-0.0482
	Н	0.5531	-0.6626	0.9491
	0	0.7612	-1.5319	-0.9203
	Н	-0.1710	-1.7936	-0.7778
	C	2.4542	-0.1802	0.0469
	Н	2.6541	0.6756	0.6949
	Н	2.9622	-1.0587	0.4495
	Н	2.8493	0.0351	-0.9491
	С	-2.0529	-0.2211	-0.4419
NHO nonovoDrolog	С	-1.0479	-1.1272	0.2020
innz_noncycrieim	С	0.9272	0.0649	-0.4132
	N	-2.0193	1.0483	-0.5199
	÷			

	Н	-2.9253	-0.7479	-0.8442
	Н	-1.4952	-2.0020	0.6842
	N	0.2213	-1.0442	0.2474
	С	2.3676	-0.3736	-0.6739
	Н	2.9253	0.4255	-1.1695
	Н	2.8613	-0.6158	0.2713
	Н	2.3908	-1.2594	-1.3143
	Н	0.4484	0.3122	-1.3702
	N	0.8047	1.2605	0.4422
	Н	-1.1615	1.4031	-0.0686
	Н	1.1634	1.0453	1.3702
	Н	1.3929	2.0020	0.0698
	С	-0.5834	-1.3914	0.7395
	С	-0.5834	-1.3914	-0.7395
	С	-0.5911	0.6649	0.0000
	Ν	-0.5886	-0.1905	1.1898
	Н	-0.5794	-2.2662	1.3808
Dero Leo	Н	-0.5794	-2.2662	-1.3808
Pieim	Ν	-0.5886	-0.1905	-1.1898
	С	0.5923	1.6356	0.0000
	Н	0.5555	2.2662	0.8890
	Н	1.5309	1.0769	0.0000
	Н	0.5555	2.2662	-0.8890
	Н	-1.5309	1.2324	0.0000
	С	-1.5859	0.3504	-0.0001
	С	-1.5379	-1.0175	-0.0007
	С	0.5171	-0.3625	-0.0005
	Ν	-0.2677	0.7549	-0.0005
	Н	-2.4019	1.0533	0.0000
2MI	Н	-2.3654	-1.7104	-0.0009
21111	N	-0.2265	-1.4543	0.0000
	C	2.0092	-0.3098	-0.0005
	Н	2.3902	0.2126	-0.8830
	Н	2.3902	0.2108	0.8830
	Н	2.4019	-1.3259	-0.0015
	Н	0.0563	1.7104	-0.0008

Table S10. Cartesian coordinates of the transition states with the participation of one water molecule

TS	Atom	X	Y	Z
	С	-2.1313	1.2791	-0.5787
	Н	-2.0731	1.9593	-1.4540
	С	-1.3188	-0.0114	-0.7240
	Н	-1.6191	-0.4422	-1.6997
	0	-1.4247	-0.8605	0.3199
	0	-2.8112	1.5376	0.3806
	0	0.6514	-1.9945	-0.1251
	Н	1.2333	-2.0539	0.6392
	Н	-0.4963	-1.5360	0.2315
CO INH2NH2CHCH3 Y	С	0.7975	1.4465	-0.1174
00+INH2INH2CHCH5_X	С	0.7273	1.0712	1.3598
	Н	1.1625	1.8830	1.9446
	Н	-0.2990	0.8965	1.6804
	Н	1.2977	0.1585	1.5429
	Ν	0.1695	0.3589	-0.9683
	Н	0.3406	0.5958	-1.9446
	Н	0.6516	-0.6154	-0.7298
	Н	0.2256	2.3583	-0.3009
	N	2.1299	1.6422	-0.6513
	Н	2.4124	2.6110	-0.5654

	Н	2.8112	1.0752	-0.1564
	Н	-0.9569	-1.6781	0.3114
	Н	-0.0530	-2.6110	-0.2297
	Н	-0.9939	-1 6473	-0.2363
	 Ц	-0.7737	-1.0475	-0.2303
	П	0.0457	-0.8079	-0.9430
	<u> </u>	-1.9178	-0.6610	-0.5905
	H	-1.9274	0.1892	-1.2846
	С	-0.6881	-0.5152	0.3308
	Н	-0.6176	-1.4171	0.9531
	N	0.5325	-0.5022	-0.5949
	Н	0 4089	-1 1953	-1 3359
	C	1 8360	0.7151	0.11/1
		1.0309	-0.7131	0.1141
	П	1.8222	-0.0077	0.9403
	C	2.9828	-0.4331	-0.8362
	H	2.9142	0.5816	-1.2322
	Н	3.9262	-0.5413	-0.3006
	Н	2.9677	-1.1438	-1.6663
	0	-0.6898	0.6302	1.0734
	Н	-0.4012	1 4418	0 2975
Bc+OHNH2CHCH3_Y	0	0.03/0	1 0085	_0 7762
		0.0349	1.770J	-0.7702
	H	0.7763	2.5/31	-0.5589
	H	0.4981	0.5307	-0.9664
	N	-3.0877	-0.7641	0.2525
	Н	-3.0121	-0.0795	0.9999
	Н	-3.9262	-0.5487	-0.2770
	0	-1.7966	-1.8145	-1.4205
	Н	-2.0053	-2.5731	-0.8582
	0	1 9257	-2 0455	0.5562
	<u></u> U	1.5257	2.0433	1.4251
	П	1.3164	-2.1242	1.4231
	H	0.0202	0.8083	1.0003
	H	-0.8297	0.9537	0.0588
	H	-0.2099	1.3033	-0.1896
	Н	-0.0638	0.1366	-1.0553
	С	-1.0679	0.5698	0.4486
	С	-0.5636	-0.3006	-0.7234
	N	0.9328	-0.2263	-0.9036
	Н	1.2239	0.8471	-0.9818
	Н	1 1741	-0 7059	-1 7702
	C	1.6200	2 0536	0.7763
		1.0200	-2.0550	0.7705
	П	1.3728	-2.8009	-0.0110
	H	0.6745	-2.0410	1.3139
	Н	2.4266	-2.3114	1.4657
	C	1.9259	-0.6809	0.2082
	Н	2.8695	-0.7110	-0.3548
	0	1.9508	0.3020	1.1781
	0	1.8942	2.0837	-0.4430
De Y	н	1 9954	1 2674	0 5730
	и	1 2005	2 8060	_0 2475
	11	0.4707	1 50007	0.24/3
	П	-0.0/9/	1.3820	0.2834
	H	-0.96/8	0.1393	-1.6389
	0	-1.0018	-1.6175	-0.5499
	H	-1.1318	-2.0279	-1.4115
	0	-0.6577	0.0898	1.7201
	Н	0.3171	0.2176	1.7702
	Ν	-2.5052	0.6087	0.3491
	н	-2 8599	-0 3316	0 5060
	<u>п</u>	2.0599	1 1002	1 0072
	П	-2.0095	1.1903	1.0972
	H	1.39/6	-0.6804	-0.11/4
	H	0.7129	0.3910	-1.0802
	Н	1.0980	-0.4100	-0.4845

	н	2 1314	1 1951	0.9391
		1 5 (5 5	1.1751	0.53/1
	H	1.3035	1.2047	-0.5240
	H	1.4977	0.8506	0.3332
	C	1.1953	-0.2840	0.7837
	Н	0.8698	-0.3985	1.8263
	С	0.5615	-1.4434	-0.0334
	Н	0.5970	-2.3822	0.5289
	0	1 2544	-1 5385	-1 2628
	0	2 5 2 2 5	-1.5505	-1.2020
	0	2.3233	-0.0080	0.0702
	0	2.4699	1.5788	-1.0829
	H	2.6604	0.6615	-0.2046
	Н	0.7319	-2.1214	-1.8263
	С	-0.8022	0.3696	-0.5579
	С	-2.1018	1.0762	-0.2303
	Н	-2 0428	2 1342	-0.4916
	 Ц	2.0120	0.6242	0.8003
X 2		-2.9130	0.0242	-0.8003
A_2	H	-2.3323	0.9881	0.8550
	N	-0.8249	-1.0607	-0.2660
	Н	-1.3877	-1.2527	0.5584
	Н	2.8702	2.3822	-0.7335
	Н	-0.5448	0.5018	-1.6094
	N	0.3754	0.9289	0.2131
	Н	1 1199	1 4319	-0 4342
	и	0.0854	1 5/180	0.0456
		0.0004	0.6529	0.2174
	П	0.8100	0.0328	0.5174
	<u>H</u>	2.9150	0.0453	-0.1730
	H	1.6819	1.2380	-0.6953
	H	2.0719	0.3403	-0.3757
	Н	0.9037	0.1532	0.6123
	Н	0.6321	0.9708	-0.6025
	С	0.6913	1.7261	-0.5025
	C	1 1789	0.8318	0 7024
	C C	1 2031	0.3886	1 2100
		0.0059	0.3000	0.1205
	п	-0.0038	2.4708	-0.1203
	H	1.4604	1.5441	1.4921
	N	-0.0097	0.8323	-1.4249
	H	0.6327	0.1938	-1.9410
	Ν	0.2240	-0.1027	1.0556
	Н	0.1952	-1.4841	0.3100
	С	-2.2968	1.0431	-0.4550
	Н	-1.9789	1.8877	0.1474
	0	2 /686	0 1005	0.2500
	<u></u>	2.7000	0.1775	0.2370
X C	П	3.0302	0.7104	-0.0140
¥_2		1./915	2.31/9	-1.13//
	H	1.4935	3.0755	-1.6533
	H	-1.4628	-0.5050	-1.7714
	Н	0.1912	-0.1962	2.0656
	0	0.1704	-2.3782	-0.2428
	Н	-0.7626	-2.5588	-0.3939
	0	1.7575	-1.1870	-2.0656
	Н	1 1566	-1 7950	-1 5711
	и	2 2401	_0 7750	_1 3109
	11	2.2401	-0.7730	-1.3170
	H	-2./081	0.3026	0.1923
	H	-3.0562	1.3659	-1.1790
	Н	0.4623	-1.0033	0.6402
	Н	-0.3447	-1.6626	-0.0844
	Н	0.7496	-3.0755	0.0136
	С	1.3437	-1.3548	0.3046
2 OH PreIm	Н	1.9341	-1.6166	1,1926
2_011_1101111	C	0.0731	-0.6678	0.7633
		0.0731	0.0070	0.1055

	Н	-0.5833	-1.0782	1.5157
	0	-1.3795	-1.1676	-0.6942
	0	1.0452	-2.5316	-0.4173
	Н	1.8688	-3.0252	-0.4973
	Н	-1 8677	-1 9232	-0 3495
	C	1.0077	0.8818	-0.5009
	C	1.1500	0.0010	-0.3009
		1.9093	2.1700	-0.2321
	H	2.0725	2.3202	-1.0204
	H	1.2236	3.0252	-0.2866
	H	2.3902	2.1530	0.7296
	N	0.1341	0.6167	0.5404
	H	-0.8537	1.0753	0.4430
	Н	0.6232	0.9391	-1.4574
	Ν	2.0159	-0.3076	-0.4637
	Н	2.9105	-0.0808	-0.0472
	0	-2.3086	0.9835	-0.0658
	Н	-2.3829	1.5296	-0.8558
	Н	-1.9436	-0 1985	-0 4489
	н	1.5150	0.7803	1 5157
	 Ц	1.0295	-0.7805	-1.5157
	11	-1.0755	0.4800	0.1074
	H	-2.9105	0.2725	0.0735
	H	-2.0439	-0.8434	-0.6790
	C	0.7449	1.0839	0.3483
	C	0.7027	2.3147	1.2009
	H	1.4924	2.9838	0.8639
	Н	-0.2635	2.8143	1.1106
	Н	0.8846	2.0495	2.2424
	Н	-0.5462	-0.8832	1.4238
	0	0.6355	-2.2833	0.3890
5 OH PreIm (with the participation of two	Н	1 4996	-1 8798	0.1172
	н	0.8797	-2 9838	1 0022
		1 3170	0.2242	0.6371
	0	2 8024	1 2961	0.0371
		2.6934	1.5001	1 2200
	П	2.0203	1.0220	-1.2390
	0	3.0043	-1.0923	-0.2014
water molecules)	H	3.0052	-0.0210	-0.3223
,	H	3.5474	-1.2438	0.5794
	N	-0.9592	-0.0155	1.0905
	Н	-1.5336	0.4538	1.7813
	Ν	0.2206	1.1372	-0.9179
	С	-1.6487	-0.2054	-0.1759
	Н	-1.6013	-1.2652	-0.4509
	С	-0.8623	0.5674	-1.2250
	Н	-1.2425	0.6064	-2.2424
	0	-2.9655	0.2955	-0.1820
	Н	-3.5474	-0.3732	0.1966
	Н	2 4561	0.6880	0.1108
	Н	2.1301	-1 6590	-0.38/17
	 Ц	2.2745	0.2065	-0.3047
		0.5055	-0.2703	0.7220
OH_PreIm_PreIm		-0.5955	0.400/	0.7339
	H	-1.3302	0.0500	1.4913
		0.3523	1.4123	0.1320
	Н	0.3090	2.4882	0.2458
	0	-2.2488	0.5883	-0.6990
	<u>H</u>	-2.9596	1.0657	-0.2550
	С	0.9439	-0.6163	-0.5047
	С	2.1692	-1.4294	-0.0978
	Н	1.9120	-2.4882	-0.0452
	Н	2.9618	-1.2929	-0.8344
	Н	2.5274	-1.1008	0.8797
	1			

	N	1.2270	0.8114	-0.5828
	Н	-2.9618	-1.9219	0.5397
	Н	0.5860	-0.9365	-1.4913
	N	-0.1626	-0.7454	0.4585
	Н	-0.9718	-1.4773	0.3314
	0	-2.3702	-1.7803	-0.2077
	Н	-2.4276	-0.5804	-0.4924
	Н	-2.3828	-0.3004	-0.9810
	Н	-1.4497	-1.7200	-0.1063
	Н	-2.4457	-2.3189	-0.9768
	Н	-2.5942	-1.1754	-0.8039
PreIm_2MI	С	1.5645	0.8964	-0.6909
	Н	2.4092	0.8003	-1.3601
	C	1.5549	1.1075	0.6886
	Н	2.3959	1.2250	1.3601
	0	0.0183	-1.7709	0.1709
	Н	0.4023	-1.8373	1.0617
	С	-0.4670	0.8768	0.0157
	С	-1.9632	1.0332	-0.0134
	Н	-2.3945	0.4862	-0.8546
	Ν	0.2751	1.1012	1.1400
	Н	-0.2023	-0.7208	-0.0283
	N	0.2840	0.7562	-1.1290
	Н	0.6732	-2.0862	-0.4743
	Н	-2.2473	2.0862	-0.1217
	Н	-2.4092	0.6641	0.9128